

ELECTRONIC SUPPLEMENTARY INFORMATION

Spontaneous surface adsorption of aqueous graphene oxide by synergy with surfactants

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This document contains all fitting parameters and sample compositions for X-ray reflectivity (XRR) datasets generated from MOTOFIT.¹ In addition, Table 1 displays the comparison of results for nested sampling of three distinct datasets using either a two-layer or three-layer model. This analysis was performed using the *refnx*² and *dynesty*³ Python computing packages.

References

- [1] Nelson, A. Co-refinement of Multiple-Contrast Neutron/X-ray Reflectivity Data using *MOTOFIT*. *J. Appl. Crystallogr.* **2006** *39*, 273–276.
- [2] Nelson, A. R., Prescott, S. W. *refnx*: neutron and X-ray reflectometry analysis in Python. *J. Appl. Crystallogr.* **2019** *52*, 193–200.
- [3] Speagle, J. S. DYNESTY: a dynamic nested sampling package for estimating Bayesian posteriors and evidences. *Mon. Notices Royal Astron. Soc.* **2020** *493*, 3132–3158.

Table S1: Fitted values and Bayesian evidence for nested sampling of two versus three layer models for three distinct GO/surfactant compositions measured by XRR. Beside each fitted values are the model bounds for that parameter where \downarrow represents the lower bound and \uparrow represents the upper bound.

[GO] mg/mL	Surfactant	[Surf.] mM	Layer 1			Layer 2			Layer 3			Evidence $\ln(Z)$	Evidence $\ln(\text{error})$
			Thickness \AA	SLD $\times 10^{-6} \text{\AA}^{-2}$	Roughness \AA	Thickness \AA	SLD $\times 10^{-6} \text{\AA}^{-2}$	Roughness \AA	Thickness \AA	SLD $\times 10^{-6} \text{\AA}^{-2}$	Roughness \AA		
0.1	OAPB	0.2	$22.9_{2\downarrow}^{30\uparrow}$	$8.5_{8.0\downarrow}^{9.0\uparrow}$	$6.7_{2\downarrow}^8\uparrow$	$14.2_{2\downarrow}^{30\uparrow}$	$11.1_{10.6\downarrow}^{11.6\uparrow}$	$5.1_{2\downarrow}^8\uparrow$	-	-	-	-24.3	0.19
0.1	OAPB	0.2	$18.1_{2\downarrow}^{30\uparrow}$	$8.5_{8.0\downarrow}^{9.0\uparrow}$	$6.6_{2\downarrow}^8\uparrow$	$8.1_{2\downarrow}^{30\uparrow}$	$9.4_{8.0\downarrow}^{11.6\uparrow}$	$5.1_{2\downarrow}^8\uparrow$	$11.7_{2\downarrow}^{30\uparrow}$	$11.1_{10.6\downarrow}^{11.6\uparrow}$	$4.7_{2\downarrow}^8\uparrow$	-25.0	0.20
1.0	TX-100	1.0	$12.4_{2\downarrow}^{30\uparrow}$	$6.8_{6.3\downarrow}^{7.3\uparrow}$	$5.5_{2\downarrow}^8\uparrow$	$23.7_{2\downarrow}^{30\uparrow}$	$11.9_{11.3\downarrow}^{12.3\uparrow}$	$6.7_{2\downarrow}^8\uparrow$	-	-	-	-22.0	0.20
1.0	TX-100	1.0	$9.0_{2\downarrow}^{30\uparrow}$	$6.8_{6.3\downarrow}^{7.3\uparrow}$	$5.8_{2\downarrow}^8\uparrow$	$9.5_{2\downarrow}^{30\uparrow}$	$10.5_{6.3\downarrow}^{12.3\uparrow}$	$5.9_{2\downarrow}^8\uparrow$	$17.5_{2\downarrow}^{30\uparrow}$	$11.9_{11.3\downarrow}^{12.3\uparrow}$	$5.2_{2\downarrow}^8\uparrow$	-22.9	0.21
1.0	C ₁₂ E ₆	1.0	$12.7_{2\downarrow}^{30\uparrow}$	$5.6_{5.1\downarrow}^{6.1\uparrow}$	$5.5_{2\downarrow}^8\uparrow$	$24.8_{2\downarrow}^{30\uparrow}$	$12.2_{11.7\downarrow}^{12.7\uparrow}$	$7.2_{2\downarrow}^8\uparrow$	-	-	-	-31.4	0.21
1.0	C ₁₂ E ₆	1.0	$9.1_{2\downarrow}^{30\uparrow}$	$5.6_{5.1\downarrow}^{6.1\uparrow}$	$5.8_{2\downarrow}^8\uparrow$	$9.8_{2\downarrow}^{30\uparrow}$	$9.8_{5.1\downarrow}^{12.7\uparrow}$	$6.4_{2\downarrow}^8\uparrow$	$19.3_{2\downarrow}^{30\uparrow}$	$12.3_{11.7\downarrow}^{12.7\uparrow}$	$5.9_{2\downarrow}^8\uparrow$	-31.9	0.22

Table S2: Fitting parameters used to model XRR datasets of GO/TX-100 systems in MOTOFIT.

[GO] mg/mL	[TX-100] mM	[NaCl] mM	Layer 1			Layer 2		
			Thickness Å	SLD $\times 10^{-6} \text{ \AA}^{-2}$	Roughness Å	Thickness Å	SLD $\times 10^{-6} \text{ \AA}^{-2}$	Roughness Å
-	10.0	-	6.7	5.5	3.2	3.8	10.9	3.1
0.1	0.1	-	4.6	7.9	7.1	9.4	10.8	4.0
0.1	0.2	-	7.1	5.4	3.7	7.4	10.8	2.9
0.1	0.5	-	4.2	6.2	4.2	10.2	11.4	4.5
0.1	1.0	-	6.5	5.1	4.3	9.6	10.2	4.3
0.5	0.5	-	4.3	6.3	4.1	9.7	11.8	6.6
0.75	0.75	-	7.4	7.6	4.7	29.1	11.2	2.2
1.0	1.0	-	10.7	6.8	5.9	25.0	11.8	7.7
1.0	5.0	-	5.8	8.0	3.7	12.3	10.3	3.1
1.0	5.0	2.0	6.2	6.5	3.2	12.1	9.7	3.1
0.5	0.5	2.0	15.5	8.4	7.3	17.3	11.8	2.3
0.5	0.5	5.0	6.4	7.2	5.8	27.9	10.8	7.6
0.5	0.5	10	4.9	6.4	3.8	32.4	11.7	4.3

Table S3: Fitting parameters used to model XRR datasets of GO/C₁₂E₆ systems in MOTOFIT.

[GO] mg/mL	[C ₁₂ E ₆] mM	Layer 1			Layer 2		
		Thickness Å	SLD $\times 10^{-6} \text{ \AA}^{-2}$	Roughness Å	Thickness Å	SLD $\times 10^{-6} \text{ \AA}^{-2}$	Roughness Å
-	1.0	7.6	5.9	3.5	11.4	10.4	4.4
0.1	0.1	4.1	6.1	4.8	18.2	10.0	4.6
0.1	0.2	5.9	5.9	4.9	11.3	10.9	5.4
0.1	0.5	6.6	7.5	5.5	10.0	10.9	6.7
0.1	1.0	5.1	6.6	4.2	13.3	10.9	6.9
0.5	0.5	9.4	5.2	3.6	8.2	12.0	3.8
0.75	0.75	2.4	5.2	7.0	23.9	10.5	5.0
1.0	0.2	9.4	7.9	5.8	24.0	12.3	4.7
1.0	0.5	12.5	7.8	6.5	21.0	12.0	5.4
1.0	1.0	12.9	5.6	5.2	24.6	12.2	7.1
1.0	2.0	10.4	6.2	4.7	24.9	10.7	5.8
1.0	5.0	4.9	6.5	7.1	18.1	10.4	4.0

Table S4: Fitting parameters used to model XRR datasets of GO/OAPB systems in MOTOFIT.

[GO] mg/mL	[OAPB] mM	Layer 1			Layer 2		
		Thickness Å	SLD $\times 10^{-6} \text{ Å}^{-2}$	Roughness Å	Thickness Å	SLD $\times 10^{-6} \text{ Å}^{-2}$	Roughness Å
-	1.0	8.8	7.3	5.7	7.0	11.0	3.8
0.025	0.05	13.4	8.0	3.4	17.0	10.6	6.2
0.05	0.1	15.8	7.3	4.2	17.3	11.0	6.1
0.1	0.05	8.8	6.9	5.5	25.1	11.8	5.6
0.1	0.1	10.2	6.8	5.9	20.8	11.5	4.5
0.1	0.2	22.2	8.5	6.6	15.7	11.1	4.9
0.1	0.5	8.5	8.6	4.8	10.7	11.5	6.5
0.2	0.4	14.8	7.5	7.1	8.9	11.2	7.1
0.5	1.0	20.2	6.9	7.7	2.2	12.0	8.0

Table S5: Fitting parameters used to model XRR datasets of GO/anionic surfactant systems in MOTOFIT.

[GO] mg/mL	Surfactant	[Surf.] mM	Layer 1			Layer 2		
			Thickness Å	SLD $\times 10^{-6} \text{ Å}^{-2}$	Roughness Å	Thickness Å	SLD $\times 10^{-6} \text{ Å}^{-2}$	Roughness Å
-	SDS	10.0	5.3	5.9	5.0	14.7	12.8	6.8
1.0	SDS	0.5	6.7	6.6	5.3	15.6	12.7	5.0
1.0	SDS	1.0	6.9	5.3	4.4	16.0	12.9	5.8
-	AOT	10.0	3.0	5.8	4.1	14.3	10.7	3.8
1.0	AOT	0.5	1.5	7.2	3.9	14.3	11.2	3.7
1.0	AOT	1.0	2.7	6.4	3.7	14.1	11.2	4.1